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1. w19_marsimpacts

1.1. Scientific Assessment

We requested HPC support to continue research on the seismic waves generated by impacts. We used the following codes: (1) **the Hybrid Optimization Software Suite (HOSS),** developed at LANL. HOSS is based on a combined Finite and Discrete Element Method (FDEM). New material models are developed for the sedimentary rocks. HOSS has been recently benchmarked to iSale and FLAG codes (Caldwell et al., 2021, accepted in Appl. Sci.); (2) **SPECFEM3D** is an open-source code developed since the last 90s. It won the Gordon Bell award for best performance in 2003, was finalist again in 2008 for a run at 0.16 petaflops on 149,784 cores on the 'Jaguar' Cray system at Oak Ridge National Laboratory (Carrington et al., 2008). It also won the BULL Joseph Fourier supercomputing award in 2010. ; (3) **SW4** is a 4th-order finite difference code developed at LLNL which is currently actively developed to handle complex 3D models and to be ported on future exascale platforms. We assessed our need to a total of 3.9M CPU-hrs for year 1 and and 3.1 M for year 2.

Achievements and Significance. This IC proposal supports the research of two CSES funded projects which aims to develop better models predicting the amplitude and shape of seismic waves generated by impacts and by coupling between Mars atmosphere and the regolith subsurface. We had two peer-review publications: (1) we publish a validation of our numerical approach for impacts in regolith, and (2) we publish a modeling of the types of signal generated by the Entry, Descent and Landing of Mars2020 and an assessment of their detectability by InSight, the mission that landed in 2018. No other team in the InSight working group has access to a numerical tool as versatile as HOSS, allowing for the first time the modeling of the shear energy generated by impacts in 3D models.

By the first publication, we reach our goal to validate the numerical approach to impact in Mars regolith which are realistic geologic material. The FDEM approach is necessary to capture the large strain deformation occurring in the bulk of the material and creation of fracture near the impact.

By this latter publication, we reach our goal to facilitate the interpretation of the seismic data return of InSight SEIS instrument. This work also led to a refinement of the scaling laws that will be used by the InSight Science Team to reach early its Science Objective to establish a new meteorite rate (Daubar et al., 2018), addressing the question of how hard do an impact needs to hit Mars to be detected by a remote seismic station. Ambiguity in the detectability of impacts result in mission operations complexities, the need for highly sensitive yet delicate seismometers, longer mission durations, and challenging data processing, storage, and transmission schemes. This work will help with the design of future missions with a seismology component and strengthen the opportunity of LANL to be a partner of such missions.

This research also supports LANL monitoring mission as we are extending and validating our numerical tools, such improving the confidence in their use to model extreme events on Earth, be they in consolidated material (typical of US and Russian nuclear tests) or in unconventional environment.

1.2. Publications

Froment, M., E. Rougier, C. S. Larmat, Z. Lei, B. Euser, S. Kedar, J. E. Richardson, T. Kawamura, and P. H. Lognonne (2020), Lagrangian-based Simulations of Hypervelocity Impact Experiments on Mars Regolith Proxy, *Geophys. Res. Lett.*, *47*(13), 475, doi:10.1029/2020GL087393.

Fernando, B. et al. (2021), Listening for the Landing: Detecting Perseverance's landing with InSight, *Earth and Space Science*, accepted. doi:10.31223/X5TC79.

1.3. Financial Impact

We got funding from LANL Center of Spaces and Earth Sciences (CSES): $180k for FY19-22, $80k for FY21 to study the seismo-acoustic signatures of the landing of Mars2020.

1.4. Highlights

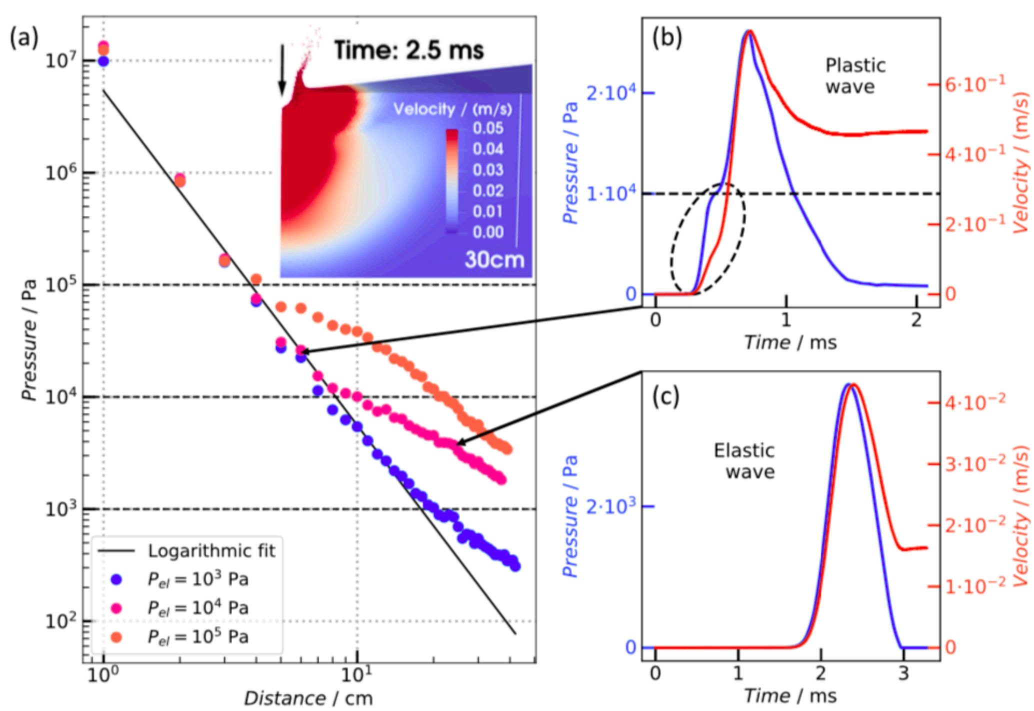

Figure 1. Evidence of an elastic and plastic regimes in our HOSS simulations of an impact of 0.29g Pyrex bead on a proxy of Mars regolith. (a) The maximum modeled pressure recorded with distance for three different values of P_{el}. In inset, a snapshot of the HOSS simulation showing the amplitude of the velocity and the ejected sand elements 2.5 ms after the impact. (b)Waveform in an area where P exceeds P_{el}=104Pa. The dashed circle indicates the elastic precursor followed by the plastic wave. (c) Waveform in

an area further away from the impact with only an elastic wave. P_{el} appears to be an important parameter controlling the transition between these two regimes.

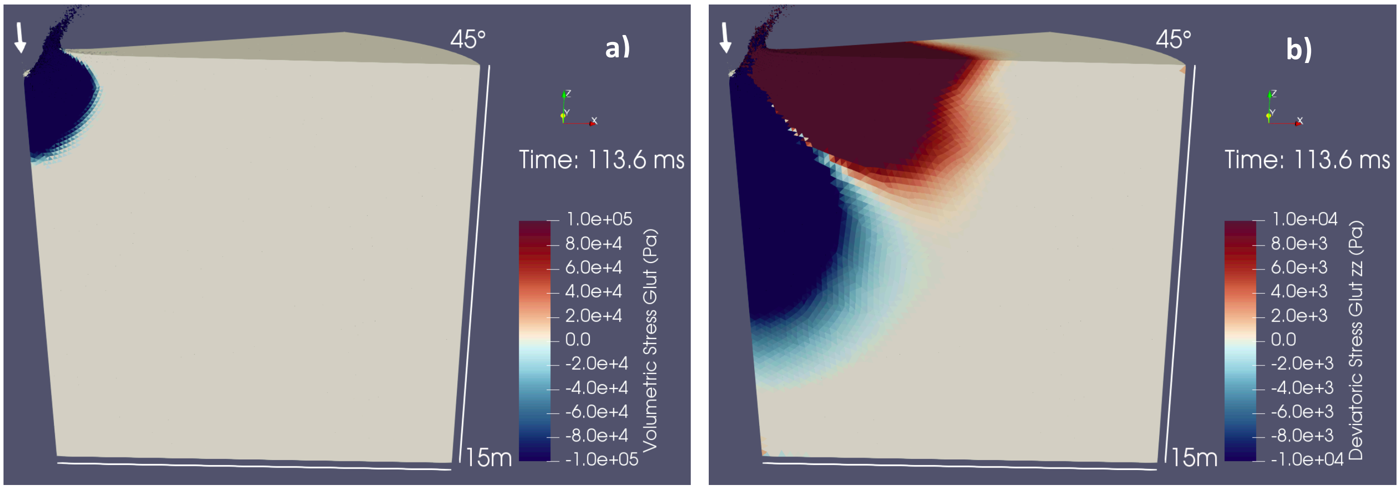

Figure 2. Volumetric (a) and vertical deviatoric (b) stress glut field (advection term ignored) generated by a 1000m/s HOSS impact simulation, after 113.6ms. Blue regions identify areas where elements were permanently compressed in volume (a) and in the z-direction (b), while red areas illustrate a permanent vertical extension. Volumetric stress glut informs on the response of the material in compression-tension (pressure) mode, when the deviatoric stress glut informs on the response in shear of the material. The latter is rarely addressed in impact modeling.

2. w19_seismicsources

2.1. Scientific Assessment

We requested HPC support to continue research on the seismic waves generated by the extreme events that are explosions. We used the following codes: (1) **the Hybrid Optimization Software Suite (HOSS),** developed at LANL. HOSS is based on a combined Finite and Discrete Element Method (FDEM). New material models are developed for the sedimentary rocks. HOSS has been recently benchmarked to iSale and FLAG codes (Caldwell et al., 2021, accepted in Appl. Sci.); (2) **SPECFEM3D** is an open-source code developed since the last 90s. It won the Gordon Bell award for best performance in 2003, was finalist again in 2008 for a run at 0.16 petaflops on 149,784 cores on the 'Jaguar' Cray system at Oak Ridge National Laboratory (Carrington et al., 2008). It also won the BULL Joseph Fourier supercomputing award in 2010. We assessed our total CPU-hours need as to 3.320M for Badger/Grizzly and 100k for Kodiak.

Achievements. When an explosion occurs underground, kinematic energy is rapidly transferred into the surrounding rock. Some volume of the rock experiences permanent deformation due to the shock waves and associated large compressive stresses happening near the explosion. We call this deformation prompt damage and it has an effect on the seismic waves generated nut the explosion. In this project, we use first principle calculations that are enabled by the coupling of HOSS to SPECFEM3D. HOSS models the dynamic nonlinear processes happening near the source, when SPECFEM3D model the propagation in realistic 3D models (Figure 3). We are currently working on the effect of prompt damage for an explosion with a scaled depth of burial of about 1600 m/kt$^{1/3}$ for which damage created by the interaction with the surface of Earth is limited. We found that even such an overburied explosion is far from the ideal isotropic compressive source model (Mueller and Murphy, 1971; Denny and Johnson, 1991) than is classically used in explosion monitoring.

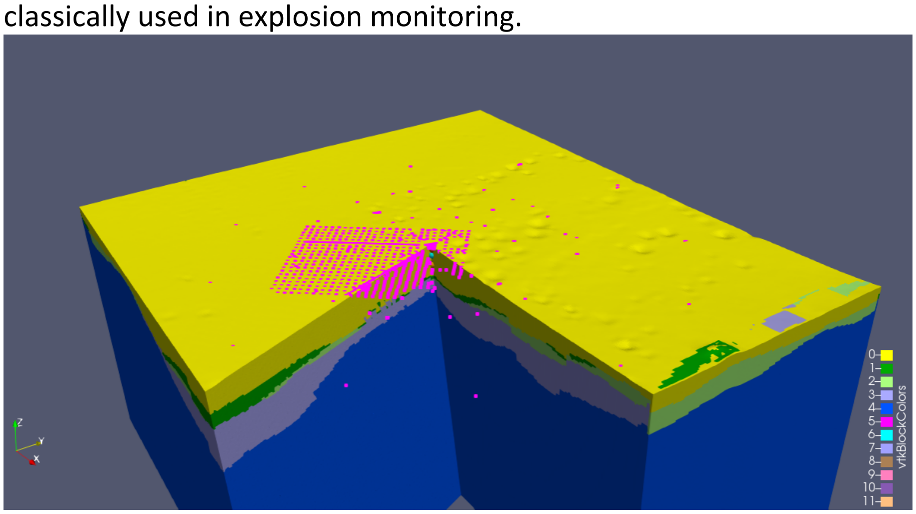

Figure 3. 3D model of a site where underground explosions were performed under the Source Physics Experiment (SPE, Snelson et al., 2013).

We also use SPECFEM3D to study how shear energy is created during the propagation of seismic waves in an realistic 3D earth model. When seismic waves encounters an interface between two different geologic units, or the free surface of earth or an heterogeneity in the subsurface, part of the wave is transmitted and reflected not in the original polarity of the wave but in the transverse. This is one of the mechanism which may explain how explosions do generate shear-wave. SPECFEM3D allows to do this type of research.

Significance. LANL is a national security science laboratory. The Lab uses science and technology to develop capabilities in response to needs of U.S. national security and to anticipate threats and enhance global security. In the last years, R&D research funded by the National Nuclear Security Administration (NNSA) in support of explosion monitoring has moved toward 3D modeling to improve knowledge of the seismic velocity structure and enable us to reduce uncertainty and more accurately detect, locate, and identify small seismic events. The proposed research supported by this Institutional Computing (IC) proposal directly addresses this goal of the NEM mission by testing and verifying the influence of geologic models to the generation of seismic waves, as well as extending current modeling capabilities to small events which are governed by different physics than bigger explosions and earthquakes. The proposed work is also supporting the SPE program of the NNSA to develop new source models for improved understanding of explosion sources. SPE R&D research has received SPE Phase-II Large Team Distinguished Performance Award in 2020 and the Secretary of Energy Achievement Honor Award of the Department of Energy for 2019 (announced January 2021).

2.2. Publications

Presentation at the 2021 Nuclear Explosion Monitoring (NEM) Program Review Meeting (March 15-19, 2021).

2.3. Financial Impact

For FY20 we got $500l from NA22 to work on the characterization of damage created by explosion. Work conducted has led to a code development effort for HOSS to conduct cratering analysis relevant to the LDRD program as well as the follow-up project with DTRA.

2.4. Highlights

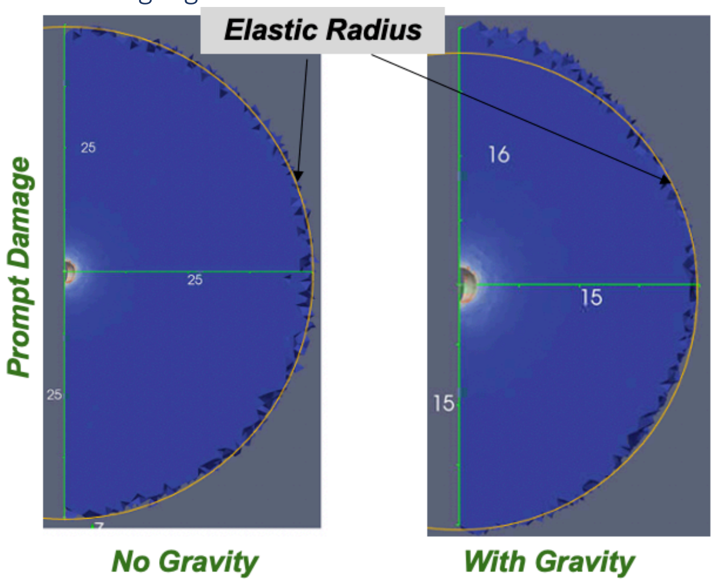

Figure 4. Volume experiencing volumetric damage modeled by HOSS for an overburied explosion. Left. Modeling without gravity; Right: Modeling with gravity introducing some anisotropy in the source.

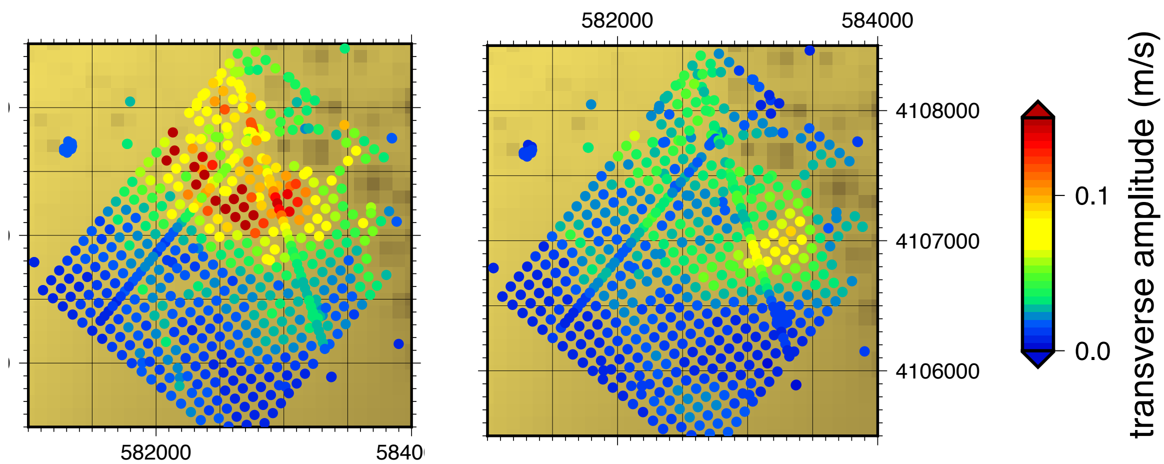

Figure 5. Low-pass amplitude (22Hz) of the modeled transverse component in two different 3D earth models with same interfaces but different elastic properties. The presence of energy on the transverse component is evidence of transfer from P to S energy of seismic waves by the 3D subsurface structure.

3. w20_gowc

3.1. Scientific Assessment

We request a one-year allocation to conduct 3D joint tomography using ambient seismic noise measurements and geodetic measurements to probe groundwater changes in Southern California. We assessed our needed resources to 80K CPU core hours on Badger, 3M CPU core hours on Grizzly and 700K GPU core hours on Kodiak.

Achievements. Increasing strains on water resources has the potential to threaten US energy production and security, as recurrent drought conditions are affecting areas that are important producers of energy, food, and other goods relying on water resources. It is important to advance monitoring methods of groundwater, especially by seeking to incorporate geophysical measurements. The latter can be done using surface sensors and satellite data in a manner more flexible and cheaper and accurate than borehole drilling. Before this research, it was shown that satellite imagery alone allows the **detection** of water loss through ground surface deformation but not necessarily **quantification** of the mass of water loss. This IC project was supporting a LDRD-ER project during which we extended advanced geophysical methods and applied them to over a decade long data holdings, especially the Los Angeles and Orange County aquifers. We use the HPC resources to seek new optimization functions for full waveform noise inversion addressing two challenges (1) seeking temporal signals in the shallow part of the Earth (less than 2km) adapting to high-frequency with local networks and (2) relatively parse data coverage.

Significance. Our results demonstrate that seismological and geophysical methods are indeed effective monitoring temporal changes in the shallow subsurface, opening the door to new applications related to energy production and water resources monitoring. In order to predict ground deformation, our joint inversion also solves for subsurface pore pressure, which is an important parameter for modeling the stress field. This connects our work to other geophysical investigations involving hazard, permeability, and reservoir management. Our results will have direct impact to the DOE cross-cutting initiative Water-Energy Nexus, DOE Geothermal, as well as the Department of Energy Office of Energy Policy and Systems Analysis (EPSA) and Biological and Environmental Research (BER) programs.

3.2. Publications

Delorey, A. A. and E. M. Syracuse. Measuring Changes in Groundwater using a Joint Inversion of Gravity and Ground Deformation. Submitted to Geophysical Research Letters. (LA-UR-20-23718)

Syracuse, E. M., J. A. Kintner, A. A. Delorey and H. Goldberg. Seismological Monitoring of Ground water Resources in the Los Angeles Region. Submitted to Journal of Geophysical Research: Solid Earth. (LA-UR-20-26268)

3.3. Financial Impact

This work led to the funding of a DOE-EERE project in 2019, entitled “Novel methods to detect small leaks” for $415k.

3.4. Highlights

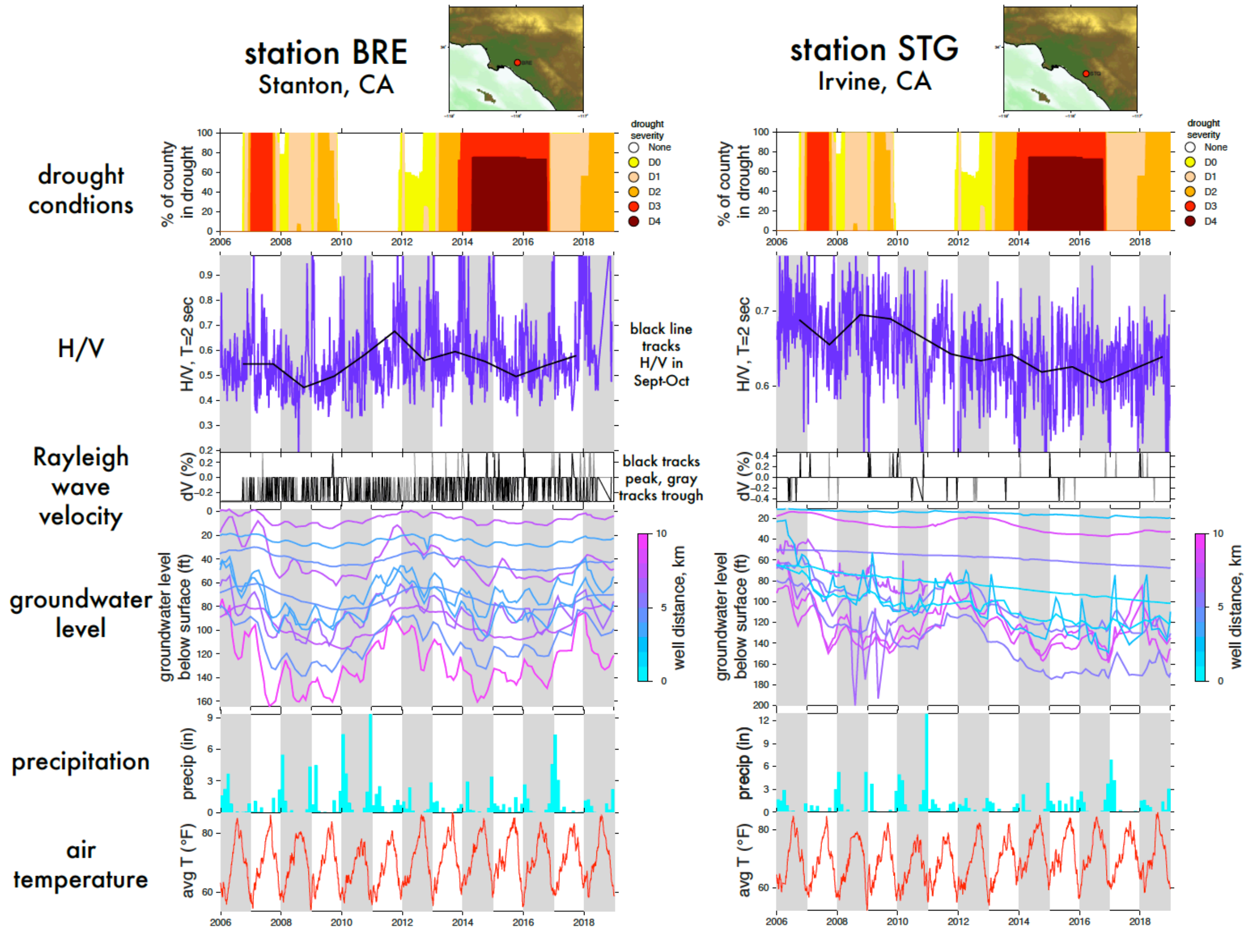

Figure 6. Seismic measurements and groundwater level correlations for two seismic stations in Southern California. The Rayleigh-wave H/V ratios exhibit positive correlation with the groundwater level changes from year 2006 to year 2019, with precipitation and air temperature also shown (Syracuse et al., submitted).

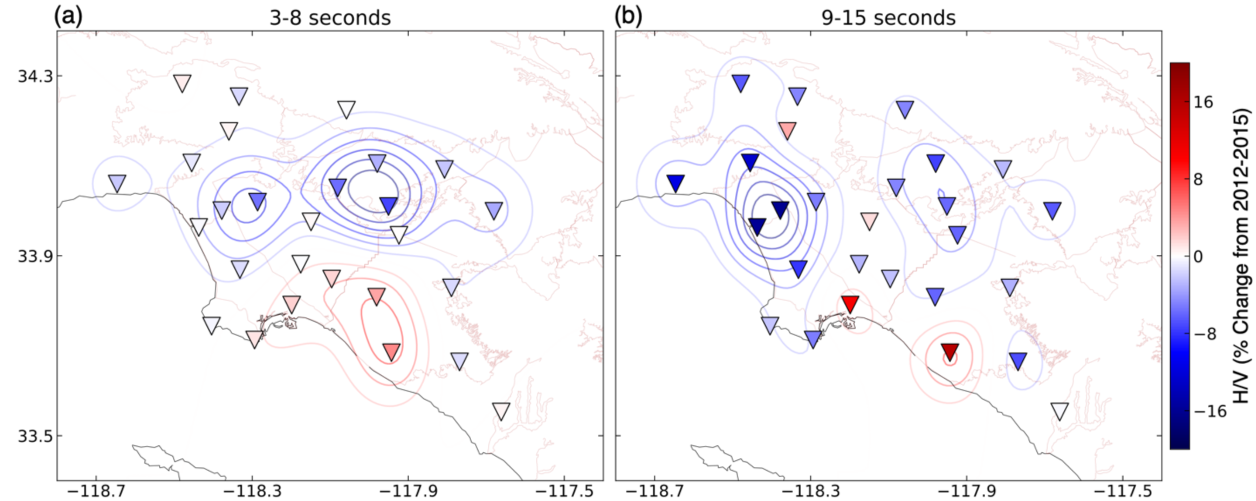

Figure 7. Percent change in H/V ratio from 2012 to 2015. Triangles and contours are colored from blue for a decrease in H/V and red to represent an increase in H/V. (a) shows the change in H/V in the 3-8 second band. (b) shows the percent change in the 9-15 second band.

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